

chain nodes :

7 8 9 10 11 12 13 14 15 16

ring nodes :

1 2 3 4 5 6

chain bonds :

1-11 2-10 3-8 4-15 5-7 6-9 11-12 11-13 11-14 12-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

3-8 5-7 11-12 12-16

exact bonds :

1-11 2-10 4-15 6-9 11-13 11-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal621con

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAPLUS F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CA/CAPLUS to MARPAT accession number crossover limit increased to 50,000
NEWS	9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	13	DEC 18	CA/CAPLUS pre-1967 chemical substance index entries enhanced with preparation role
NEWS	14	DEC 18	CA/CAPLUS patent kind codes updated
NEWS	15	DEC 18	MARPAT to CA/CAPLUS accession number crossover limit increased to 50,000
NEWS	16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	17	DEC 27	CA/CAPLUS enhanced with more pre-1907 records
NEWS	18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	19	JAN 16	CA/CAPLUS Company Name Thesaurus enhanced and reloaded
NEWS	20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	22	JAN 22	CA/CAPLUS updated with revised CAS roles
NEWS	23	JAN 22	CA/CAPLUS enhanced with patent applications from India
NEWS	24	JAN 29	PHAR reloaded with new search and display fields
NEWS	25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	26	FEB 13	CASREACT coverage to be extended
NEWS	27	Feb 15	PATDPASPC enhanced with Drug Approval numbers
NEWS	28	Feb 15	RUSSIAPAT enhanced with pre-1994 records
NEWS	29	Feb 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS	30	Feb 26	MEDLINE reloaded with enhancements
NEWS	31	Feb 26	EMBASE enhanced with Clinical Trial Number field
NEWS	32	Feb 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS	33	Feb 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS	34	Feb 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:02:20 ON 13 MAR 2007

=> FILE REG	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.63	0.63

FILE 'REGISTRY' ENTERED AT 09:04:01 ON 13 MAR 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3  
DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\TJ-1.str

L1 STRUCTURE UPLOADED

=> D L1  
L1 HAS NO ANSWERS  
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> S L1 FULL  
FULL SEARCH INITIATED 09:05:18 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 50557 TO ITERATE

100.0% PROCESSED 50557 ITERATIONS  
SEARCH TIME: 00.00.01

21 ANSWERS

L2 21 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

173.00

173.63

FILE 'CAPLUS' ENTERED AT 09:05:31 ON 13 MAR 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 13 Mar 2007 VOL 146 ISS 12

FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> S L2

L3 10 L2

=> D L4 IBIB ABS HITSTR 1-10

L4 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> D L3 IBIB ABS HITSTR 1-10

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:48551 CAPLUS

DOCUMENT NUMBER: 144:139035

TITLE: Optically active phenylenediamines, and their polyimides or polyimide precursors

INVENTOR(S): Sahade, Daniel Antonio; Oda, Takuo

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006016303	A	20060119	JP 2004-187213	20040625
PRIORITY APPLN. INFO.:			JP 2004-164336	A 20040602

OTHER SOURCE(S): MARPAT 144:139035

AB The phenylenediamines are PX1X2OG or PX1(CH2)nOX2OG [P = diaminophenyl; X1 = O, CH2O, CO2; X2 = phenylene, diphenylene; G = (R)- or (S)-X3C\*HX6X4X5; \* = chiral point; X3 = single bond, CH2; x4 = CH2, CO2; X5 = C1-10 alkyl; X6 = CF3, Me; n = 1-10]. The polyimides or polyimide precursors bearing optically active groups on side chains are useful for liquid crystal alignment films for displays.

IT 873691-16-8P

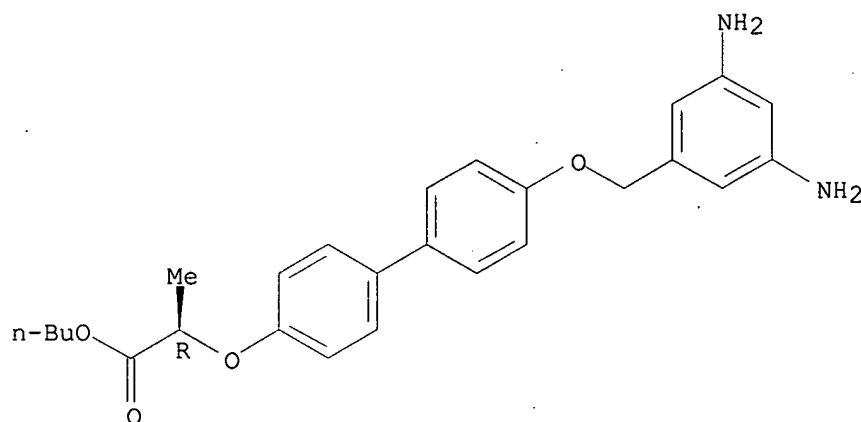
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(optically active phenylenediamines for polyimides or polyimide precursors for liquid crystal alignment films)

RN 873691-16-8 CAPLUS

CN Propanoic acid, 2-[[4'-[(3,5-diaminophenyl)methoxy][1,1'-biphenyl]-4-yl]oxy]-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 873691-26-0P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(optically active phenylenediamines for polyimides or polyimide precursors for liquid crystal alignment films)

RN 873691-26-0 CAPLUS

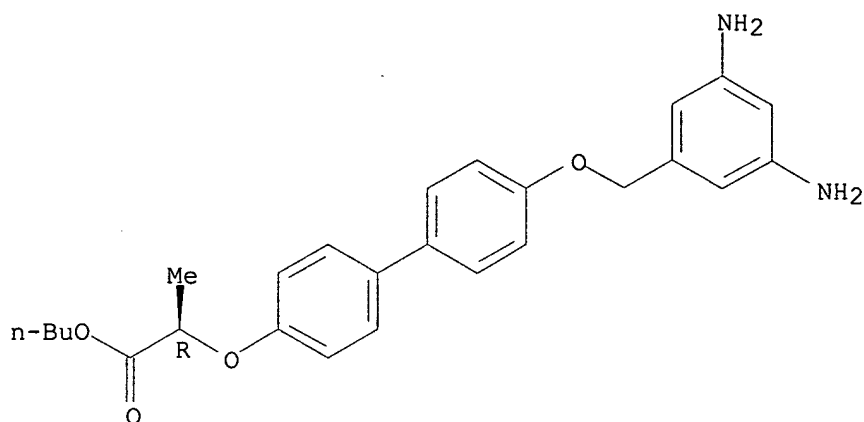
CN Propanoic acid, 2-[[4'-[(3,5-diaminophenyl)methoxy][1,1'-biphenyl]-4-yl]oxy]-, butyl ester, (2R)-, polymer with tetrahydrocyclobuta[1,2-c:3,4-c']difurantetrone (9CI) (CA INDEX NAME)

CM 1

CRN 873691-16-8

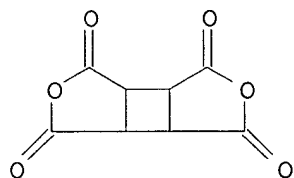
CMF C26 H30 N2 O4

Absolute stereochemistry.



CM 2

CRN 4415-87-6  
CMF C8 H4 O6



L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:996247 CAPLUS  
 DOCUMENT NUMBER: 141:429761  
 TITLE: Alignment agent for liquid crystal  
 INVENTOR(S): Taki, Hirotsugu; Saito, Tetsuya  
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan  
 SOURCE: PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099289	A1	20041118	WO 2004-JP6275	20040430
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

CN 1784452 A 20060607 CN 2004-80012064 20040430

PRIORITY APPLN. INFO.: JP 2003-129091 A 20030507

AB An alignment agent for a liquid crystal which contains one or more polymers for forming an alignment film for a liquid crystal, characterized in that at

least one of the polymers is a polymer which has an alkylene group having 4 to 16 carbon atoms in the main chain thereof and has a side chain having a function to enhance the pretilt angle of the liquid crystal. The alignment agent for a liquid crystal can provide an alignment film which allows the achievement of a high and thermally stable crystal orientation and pretilt angle without the reliance on a process, such as rubbing and cleaning by an organic solvent.

IT 796853-43-5P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
(polyimide alignment agent for liquid crystal display element)

RN 796853-43-5 CAPLUS

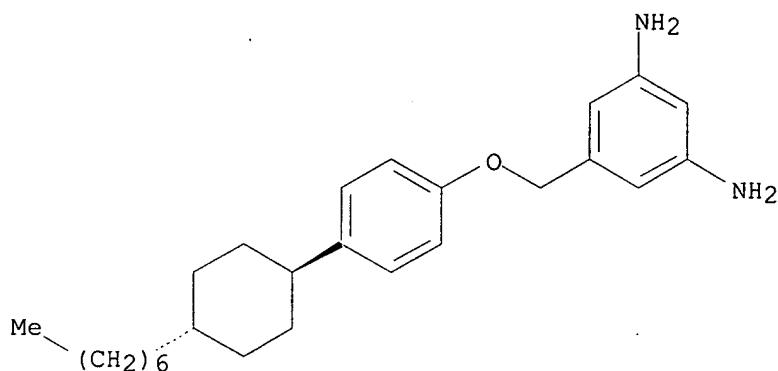
CN 1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, polymer with  
5-[[4-(trans-4-heptylcyclohexyl)phenoxy]methyl]-1,3-benzenediamine and  
4,4'-[1,5-pentanediy]bis(oxy)]bis[benzenamine] (9CI) (CA INDEX NAME)

CM 1

CRN 796853-39-9

CMF C26 H38 N2 O

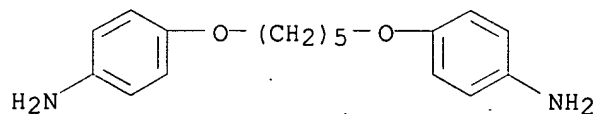
Relative stereochemistry.



CM 2

CRN 2391-56-2

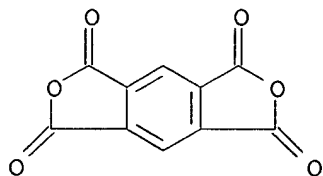
CMF C17 H22 N2 O2



CM 3

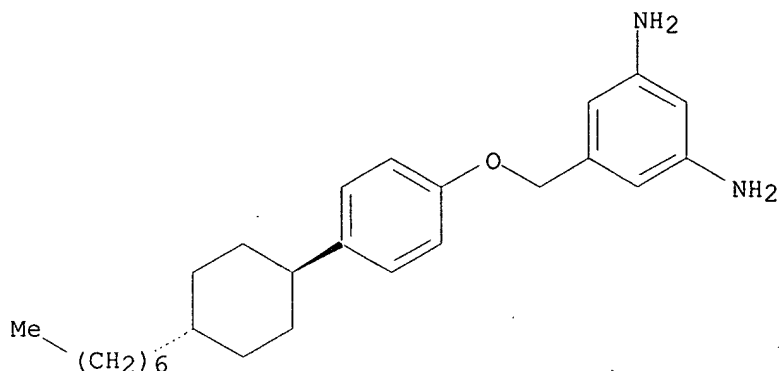
CRN 89-32-7

CMF C10 H2 O6



IT 796853-39-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (polyimide alignment agent for liquid crystal display element)  
 RN 796853-39-9 CAPLUS  
 CN 1,3-Benzenediamine, 5-[[4-(trans-4-heptylcyclohexyl)phenoxy]methyl]- (9CI)  
 (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:515568 CAPLUS

DOCUMENT NUMBER: 141:54799

TITLE: Novel diaminobenzene derivative, polyimide precursor and polyimide obtained therefrom, and aligning agent for liquid crystal

INVENTOR(S): Hosaka, Kazuyoshi; Taki, Hirotsugu; Nawata, Hideyuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

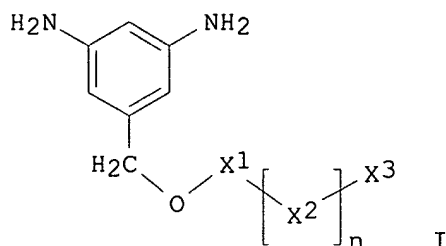
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052962	A1	20040624	WO 2003-JP15800	20031210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003289305	A1	20040630	AU 2003-289305	20031210
CN 1720280	A	20060111	CN 2003-80105205	20031210
US 2006246230	A1	20061102	US 2005-538060	20050609
PRIORITY APPLN. INFO.:			JP 2002-359224	A 20021211
			WO 2003-JP15800	W 20031210

OTHER SOURCE(S): MARPAT 141:54799

GI





AB The present invention relates to (i) a novel diamine useful especially as a material for a resin for liquid-crystal alignment films, (ii) a polyimide precursor or polyimide synthesized from the diamine, and (iii) an aligning agent for liquid crystals which comprises the polymer. The aligning agent gives a liquid-crystal alignment film which has a high pretilt angle for liquid crystals, has excellent thermal stability of the pretilt angle, and is reduced in the dependence of the pretilt angle on rubbing pressure. The diamine is a diaminobenzene derivative I, wherein X1, X2 = a cyclic group and X3 = a member selected from alkyl, alkoxy, fluoroalkyl, fluoroalkoxy, fluorine, chlorine, bromine, and cyano. The polyimide precursor or polyimide is synthesized using the diaminobenzene derivative as part of the starting materials. The aligning agent for liquid crystals comprises at least one of these polymers. Thus, 100.00 g biphenol and 103.90 g 1-bromooctane were reacted at 110° for 10 h, reacted with 3,5-dinitrobenzyl chloride, and reduced to give a diamine with m.p. 192-196°, 1.64 g of which was polymerized with 2.25 g 1,4-diaminobenzene and 7.81 g 3,4-dicarboxy-1,2,3,4-tetrahydro-1-naphthalene succinic dianhydride to give 20%-solids polyimide precursor with viscosity 3481 mPa-s and weight average mol. weight 134,600, the resulting precursor solution was diluted with NMP and Bu cellosolve, applied on an ITO-coated glass substrate, heated at 80° for 5 min and 220° for 1 h, rubbed with a rayon cloth, and fabricated into a liquid crystal cell; showing free tilt angle 6.8° initially, 6.9° after treatment at 120° for 5 min, and 6.9° after treatment at 120° for 1 h.

IT 709031-69-6P 709031-71-0P

RL: DEV (Device component use); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)

(liquid crystal; preparation of diaminobenzene derivs. for polyimide precursors useful as aligning agents for liquid crystals)

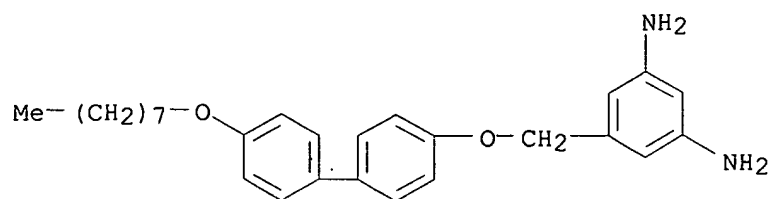
RN 709031-69-6 CAPLUS

CN Naphtho[1,2-c]furan-1,3-dione, 3a,4,5,9b-tetrahydro-5-(tetrahydro-2,5-dioxo-3-furanyl)-, polymer with 1,4-benzenediamine and 5-[[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]oxy]methyl]-1,3-benzenediamine (9CI) (CA INDEX NAME)

CM 1

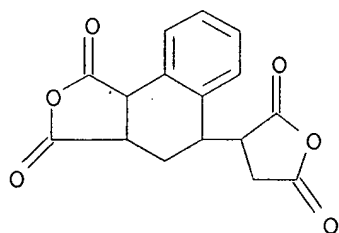
CRN 709031-65-2

CMF C27 H34 N2 O2



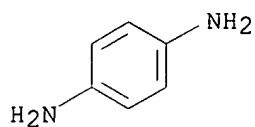
CM 2

CRN 13912-65-7  
CMF C16 H12 O6



CM 3

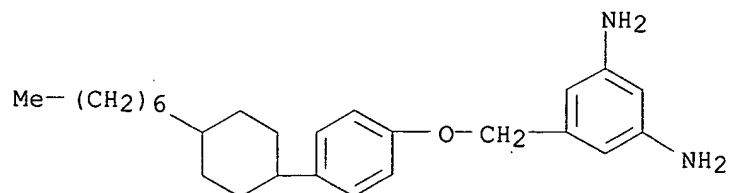
CRN 106-50-3  
CMF C6 H8 N2



RN 709031-71-0 CAPLUS  
CN Naphtho[1,2-c]furan-1,3-dione, 3a,4,5,9b-tetrahydro-5-(tetrahydro-2,5-dioxo-3-furanyl)-, polymer with 1,4-benzenediamine and  
5-[[4-(4-heptylcyclohexyl)phenoxy]methyl]-1,3-benzenediamine (9CI) (CA  
INDEX NAME)

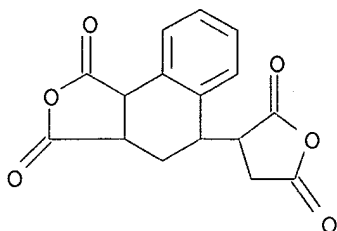
CM 1

CRN 709031-68-5  
CMF C26 H38 N2 O



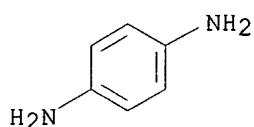
CM 2

CRN 13912-65-7  
CMF C16 H12 O6

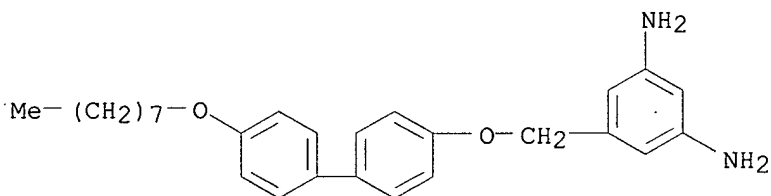


CM 3

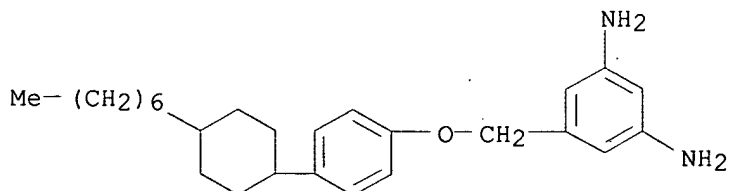
CRN 106-50-3  
CMF C6 H8 N2



IT 709031-65-2P 709031-68-5P  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
(Reactant or reagent)  
(monomer; preparation of diaminobenzene derivs. for polyimide precursors  
useful as aligning agents for liquid crystals)  
RN 709031-65-2 CAPLUS  
CN 1,3-Benzenediamine, 5-[[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]oxy]methyl]-  
(9CI) (CA INDEX NAME)



RN 709031-68-5 CAPLUS  
CN 1,3-Benzenediamine, 5-[[[4-(4-heptylcyclohexyl)phenoxy]methyl]- (9CI) (CA  
INDEX NAME)

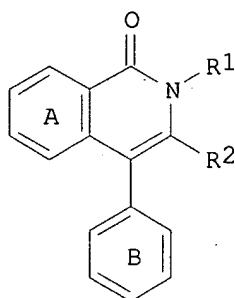


L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:902258 CAPLUS

DOCUMENT NUMBER: 137:379992  
 TITLE: Method of inhibiting neoplastic cells with  
 isoquinolinonecarboxylates  
 INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.  
 PATENT ASSIGNEE(S): Cell Pathways, Inc., USA  
 SOURCE: U.S., 119 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6486155	B1	20021126	US 1998-198413	19981124
PRIORITY APPLN. INFO.:			US 1998-198413	19981124
OTHER SOURCE(S):	MARPAT	137:379992		

GI



- AB A method is claimed for inhibiting neoplasia (no data), particularly cancerous and precancerous lesions, by exposing the affected cells to 1-isoquinoline-3-carboxylates. Such compds. are effective in modulating apoptosis and eliminating and inhibiting the growth of neoplasias such as precancerous lesions, but are not characterized by the severe side reactions of conventional non-steroidal antiinflammatory drugs or other chemotherapeutics. Although the methods of preparation are not claimed, example preps. of 429 isoquinolines and 107 intermediates are included; these examples are referenced to PCT application WO 98/38168. Although the claims indicate I (ring A and ring B are the same or different and each a (un)substituted benzene ring, R1 is morpholine, R2 is -COOR3, and R3 is alkyl; e.g. 7-benzyloxy-6-methoxy-3-methoxycarbonyl-2-morpholino-4-(3,4,5-trimethoxyphenyl)-1(2H)-isoquinolinone) or pharmaceutically acceptable salt thereof, the examples include a much broader variety of 1-isoquinoline-3-carboxylates.
- IT 212498-74-3P, 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride 212499-20-2P, 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride 212499-85-9P, 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester, trihydrochloride 212500-32-8P, 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester 212500-49-7P, 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester 212500-73-7P, 3-Isoquinolinecarboxylic acid,

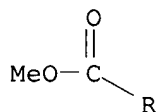
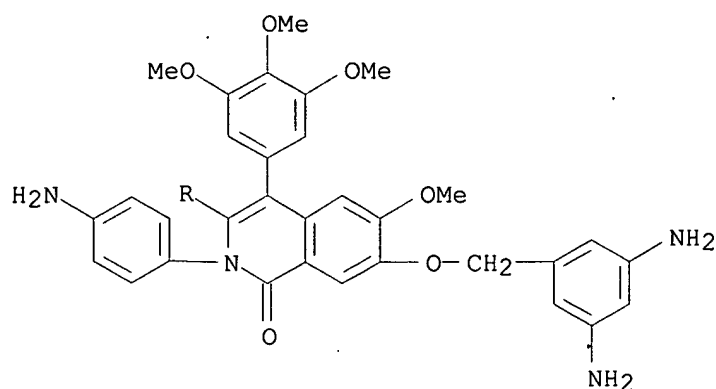
2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester  
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of isoquinolinonecarboxylates for inhibiting neoplastic cells)

RN 212498-74-3 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

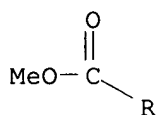
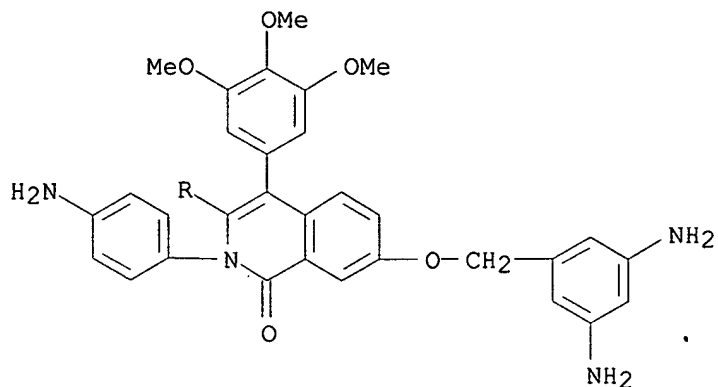


PAGE 2-A

● 3 HCl

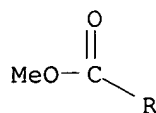
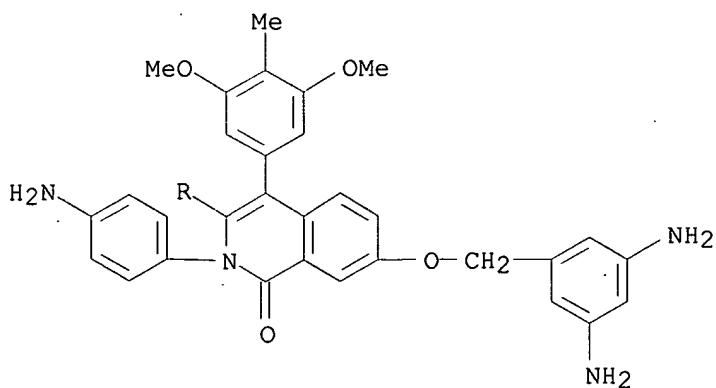
RN 212499-20-2 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)



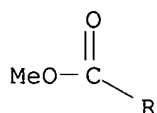
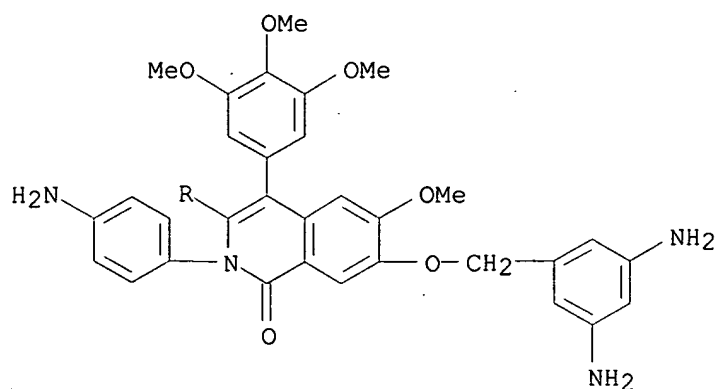
● 3 HCl

RN 212499-85-9 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester, trihydrochloride (9CI). (CA INDEX NAME)

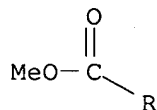
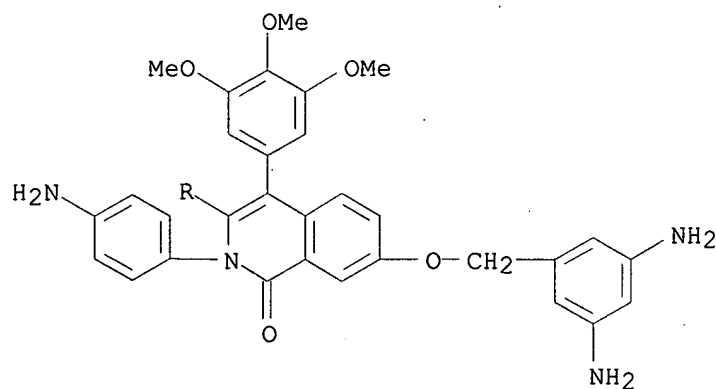


● 3 HCl

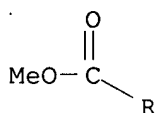
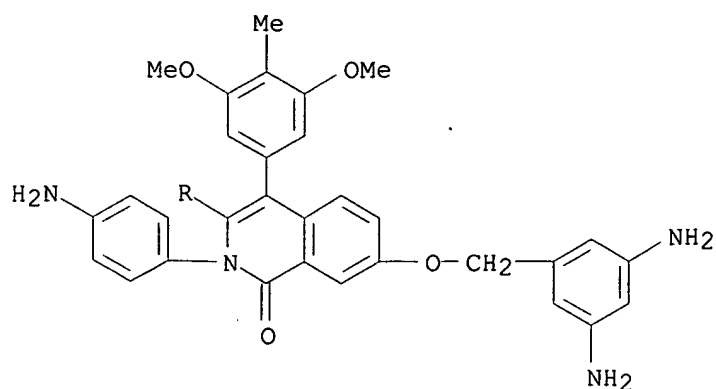
RN 212500-32-8 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 212500-49-7 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 212500-73-7 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 171 THERE ARE 171 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:575044 CAPLUS

DOCUMENT NUMBER: 137:124993

TITLE: Trisubstituted carbocyclic cyclophilin binding compounds and their use

INVENTOR(S): Wu, Yong-Qian; Belyakov, Sergei; Hamilton, Gregory; Limburg, David; Steiner, Joseph; Vaal, Mark; Wei, Ling; Wilkinson, Douglas

PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002059080	A2	20020801	WO 2002-US2538	20020125
WO 2002059080	A3	20021219		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2435829	A1	20020801	CA 2002-2435829	20020125
US 2002165275	A1	20021107	US 2002-57203	20020125
US 6656971	B2	20031202		
EP 1360173	A2	20031112	EP 2002-706049	20020125
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004532187	T	20041021	JP 2002-559382	20020125



US 2004157919  
PRIORITY APPLN. INFO.:

A1 20040812

US 2003-713566 20031114  
US 2001-263703P P 20010125  
US 2001-291965P P 20010521  
US 2001-291365P P 20010517  
US 2002-57203 A3 20020125  
WO 2002-US2538 W 20020125

OTHER SOURCE(S): MARPAT 137:124993

AB Novel, non-peptidic small organic compds. having an affinity for cyclophilin (CyP)-type immunophilin proteins are reported. These compds. are used for binding CyP-type proteins, inhibiting their peptidyl-prolyl isomerase activity. Thus, 5-HOC6H3(CO2Me)2-1,3 was O-benzylated, hydrolyzed to the acid and treated with 3,4-Cl2C6H3NH2 to give 5-PhCH2OC6H3(CONHC6H3Cl2-3,4)2-1,3. This compound gave complete protection against cell death in L-threo-3-hydroxyaspartic acid treated spinal cord slices.

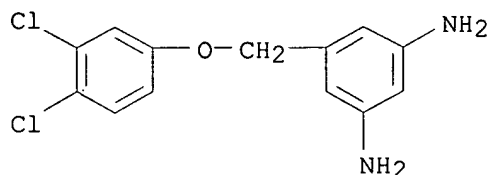
IT 444343-54-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(trisubstituted carbocyclic cyclophilin binding compds.)

RN 444343-54-8 CAPLUS

CN 1,3-Benzenediamine, 5-[(3,4-dichlorophenoxy)methyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:151451 CAPLUS

DOCUMENT NUMBER: 132:207769

TITLE: Preparation of isoquinolinones as effective component in medicine

INVENTOR(S): Ukita, Shinzo; Ohmori, Kanji; Ikeo, Tomihiro

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 148 pp.

CODEN: JKXXAF

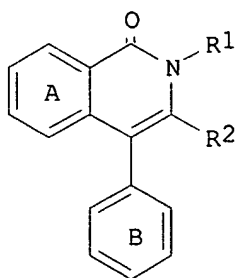
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

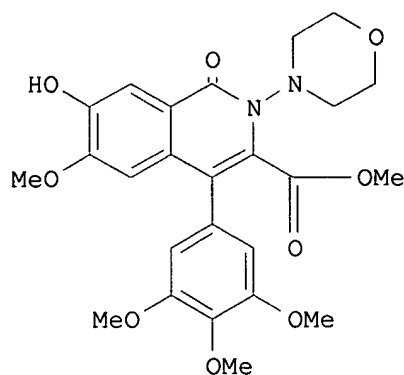
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000072675	A	20000307	JP 1998-240446	19980826
PRIORITY APPLN. INFO.:			JP 1998-240446	19980826
OTHER SOURCE(S):	MARPAT 132:207769			
GI				



I



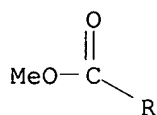
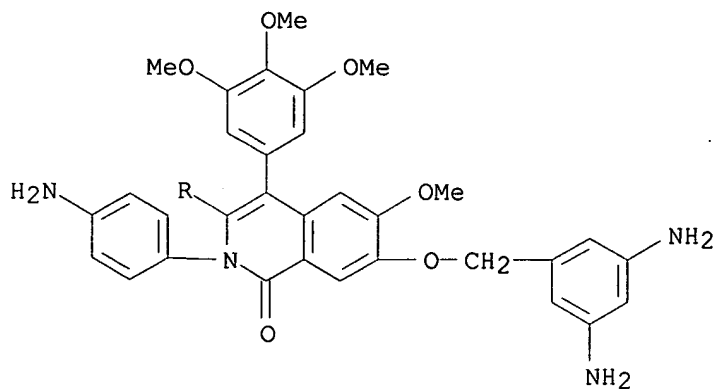
II

AB Title compds. [I; ring A and ring B equivalent or different, substituted or unsubstituted benzene ring; R1 = H, N(CH3)2, 4-H2NC6H4, 4-CH3OCOC6H4, alkyl, cycloalkyl, aryl, complex cyclic; R2 = COOH, COOCH3, COOCH2CH3, COOCH2C6H5, COO(CH2)3CH3] and pharmaceutical acceptable salts are prepared and tested as PDEV inhibitors. The title compound II was prepared

IT 212498-74-3P 212499-20-2P 212499-85-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of isoquinolinones as effective component in medicine)

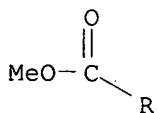
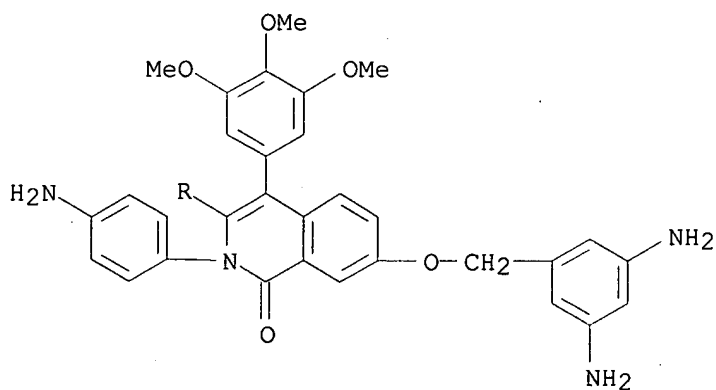
RN 212498-74-3 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

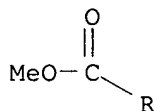
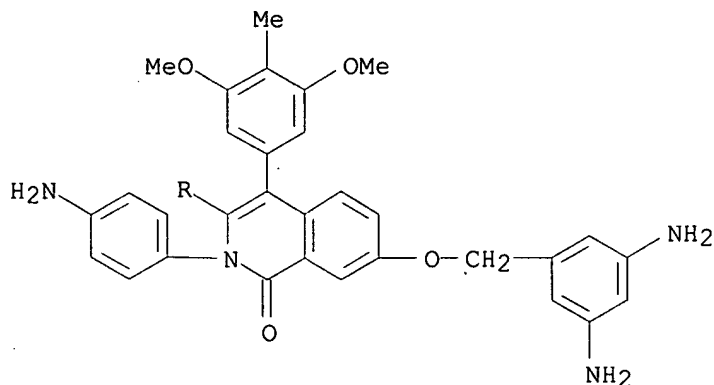
RN 212499-20-2 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

RN 212499-85-9 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

● 3 HCl

L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1998:608601 CAPLUS  
 DOCUMENT NUMBER: 129:216521  
 TITLE: Preparation of 1-isoquinolinone-3-carboxylates as PDE V inhibitors  
 INVENTOR(S): Ukita, Tatsuzo; Omori, Kenji; Ikee, Tomihiro  
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 299 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9838168	A1	19980903	WO 1998-JP715	19980223
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1998MA00345	A	20050304	IN 1998-MA345	19980220
AU 9862300	A	19980918	AU 1998-62300	19980223

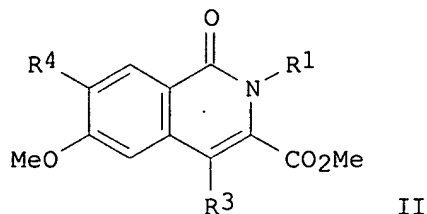
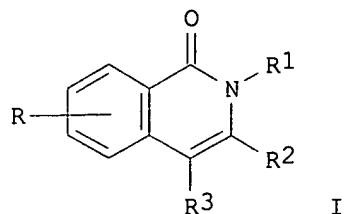
JP 10298164  
PRIORITY APPLN. INFO.:

A 19981110  
MARPAT 129:216521

JP 1998-44139  
JP 1997-44408  
WO 1998-JP715

19980226  
A 19970227  
W 19980223

OTHER SOURCE(S):  
GI



AB Title compds. [I; R = H or substituent(s); R1 = H, NH2, (cyclo)alkyl, heterocyclyl, aryl, etc.; R2 = (esterified) CO2H, CONH2, N-attached heterocyclylcarbonyl, etc.; R3 = (un)substituted Ph] were prepared as PDE V inhibitors (no data). Thus, 5-benzyloxy-4-methoxy-2-(3,4,5-trimethoxybenzoyl)benzoic acid was cyclocondensed with CH2(CO2CMe3)2 and the hydrated product cyclocondensed with 4-(H2N)C6H4NHCOCMe3 to give, in 4 addnl. steps, title compound II [R1 = C6H4(NH2)-4, R3 = C6H2(OMe)3-3,4,5, R4 = 2-pyridylmethoxy].

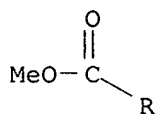
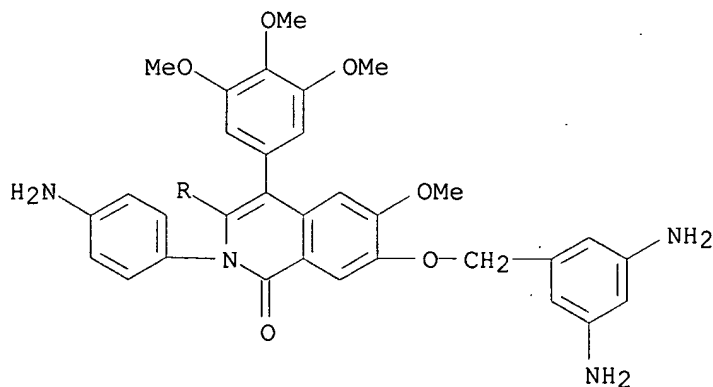
IT 212498-74-3P 212499-20-2P 212499-85-9P  
212500-32-8P 212500-49-7P 212500-73-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of 1-isoquinolinone-3-carboxylates as PDE V inhibitors)

RN 212498-74-3 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)

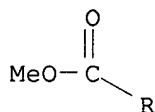
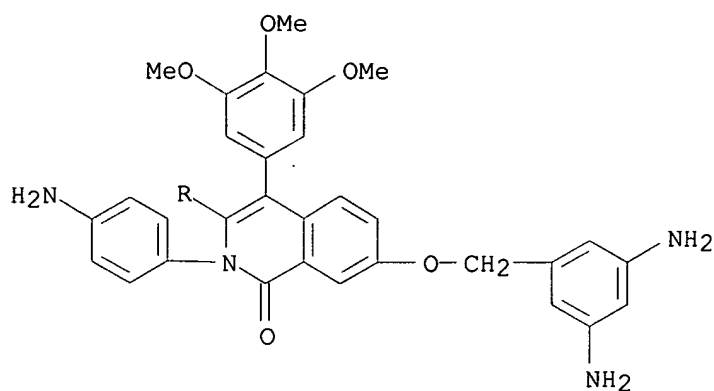
PAGE 1-A



● 3 HCl

RN 212499-20-2 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)

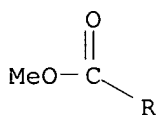
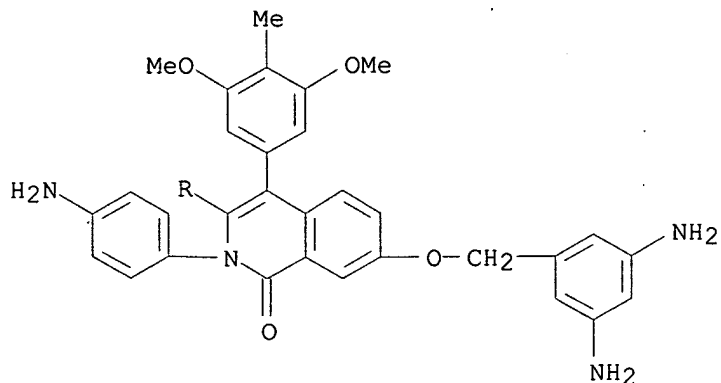
PAGE 1-A



PAGE 2-A

● 3 .HCl

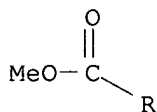
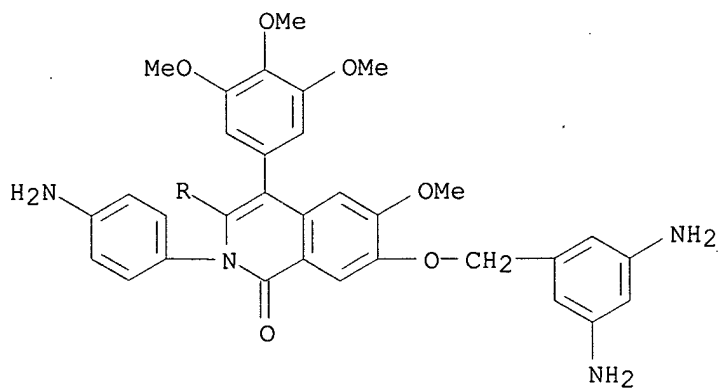
RN 212499-85-9 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

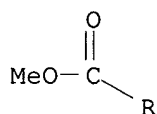
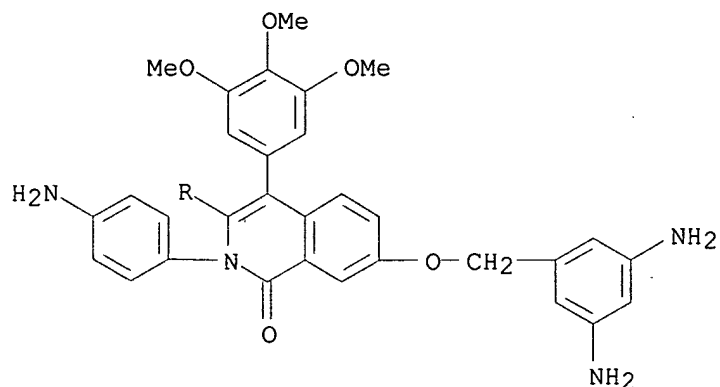
RN 212500-32-8 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-6-methoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

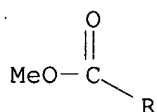
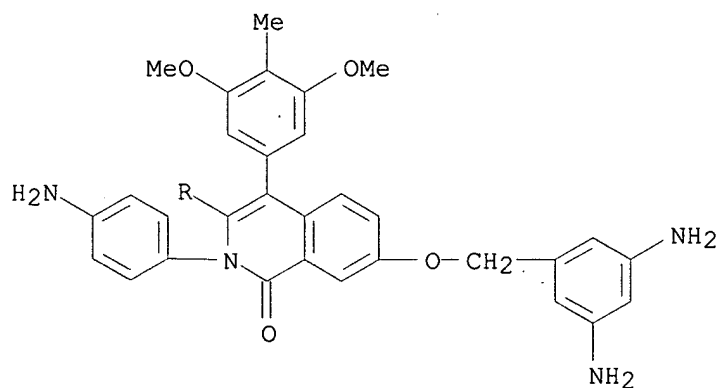


RN 212500-49-7 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-1,2-dihydro-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 212500-73-7 CAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 2-(4-aminophenyl)-7-[(3,5-diaminophenyl)methoxy]-4-(3,5-dimethoxy-4-methylphenyl)-1,2-dihydro-1-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:247213 CAPLUS  
 DOCUMENT NUMBER: 125:34617  
 TITLE: An analysis of relaxation processes in electro-optic polymers  
 AUTHOR(S): Burland, Donald M.; Verbiest, Thierry  
 CORPORATE SOURCE: Res. Div., IBM, San Jose, CA, USA  
 SOURCE: MCLC S&T, Section B: Nonlinear Optics (1996), 15(1-4),



299-306

CODEN: MCLOEB; ISSN: 1058-7268

PUBLISHER:

Gordon & Breach

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The orientational relaxation of dipolar chromophores dissolved in or attached to an amorphous polymer was studied by monitoring the decay of the 2nd-harmonic generation. From the temperature dependence of the fitting parameters associated with the log-normal or Wagner function activation, the entropies, enthalpies, and thermal expansion coeffs. were determined

IT 177994-71-7 177994-72-8

RL: PRP (Properties)

(anal. of orientational relaxation of dipolar chromophores dissolved in or attached to amorphous polymers)

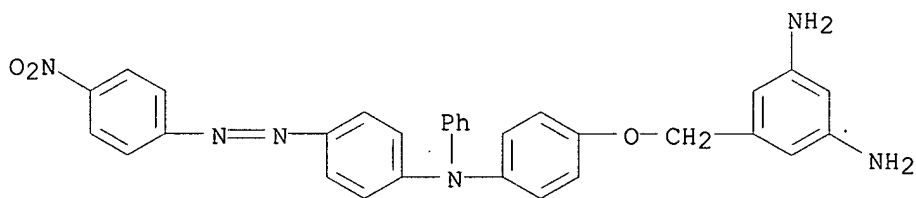
RN 177994-71-7 CAPLUS

CN 1,3-Isobenzofurandione, 5,5'-oxybis-, polymer with 5-[[4-[[4-[(4-nitrophenyl)azo]phenyl]phenylamino]phenoxy]methyl]-1,3-benzenediamine (9CI) (CA INDEX NAME)

CM 1

CRN 177994-70-6

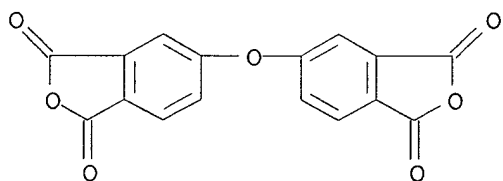
CMF C31 H26 N6 O3



CM 2

CRN 1823-59-2

CMF C16 H6 O7



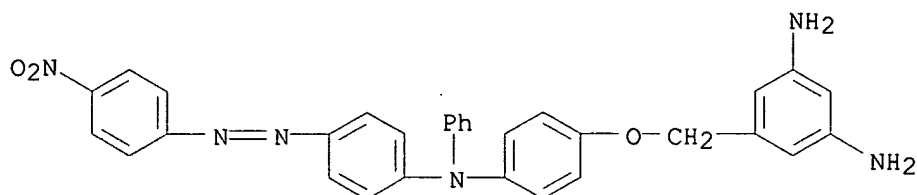
RN 177994-72-8 CAPLUS

CN 1,3-Isobenzofurandione, 5,5'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis-, polymer with 5-[[4-[[4-[(4-nitrophenyl)azo]phenyl]phenylamino]phenoxy]methyl]-1,3-benzenediamine (9CI) (CA INDEX NAME)

CM 1

CRN 177994-70-6

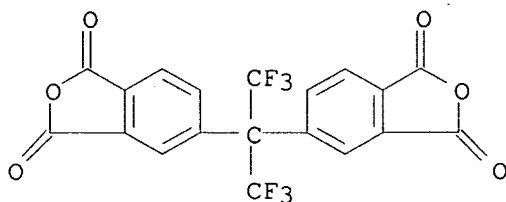
CMF C31 H26 N6 O3



CM 2

CRN 1107-00-2

CMF C19 H6 F6 O6



L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:969418 CAPLUS

DOCUMENT NUMBER: 124:202946

TITLE: Preparation of sulfate esters of sugar alcohols for the treatment of arteriosclerotic changes in the vascular walls.

INVENTOR(S): Chucholowski, Alexander; Fingerle, Juergen; Iberg, Niggi; Maerki, Hans Peter; Mueller, Rita; Pech, Michael; Rouge, Marianne; Schmid, Gerard; Tschopp, Thomas; Wessel, Hans Peter

PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.

SOURCE: Eur. Pat. Appl., 42 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 663391	A1	19950719	EP 1995-100180	19950109
EP 663391	B1	19970409		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5521160	A	19960528	US 1995-368519	19950104
CA 2139720	A1	19950715	CA 1995-2139720	19950106
ZA 9500086	A	19950720	ZA 1995-86	19950106
AU 9510106	A	19950727	AU 1995-10106	19950109
AU 685196	B2	19980115		
HU 72412	A2	19960429	HU 1995-52	19950109
AT 151416	T	19970415	AT 1995-100180	19950109
ES 2101583	T3	19970701	ES 1995-100180	19950109
IL 112284	A	19981030	IL 1995-112284	19950109
FI 9500127	A	19950715	FI 1995-127	19950111
CN 1109889	A	19951011	CN 1995-101166	19950111
CN 1043349	B	19990512		
RU 2139854	C1	19991020	RU 1995-100773	19950111
NO 9500137	A	19950717	NO 1995-137	19950113
JP 07206803	A	19950808	JP 1995-3729	19950113

JP 2862489 B2 19990303  
 PL 180273 B1 20010131 PL 1995-306797 19950113  
 BR 9500096 A 19951031 BR 1995-96 19951013  
 PRIORITY APPLN. INFO.: CH 1994-114 A 19940114  
 CH 1994-3315 A 19941107

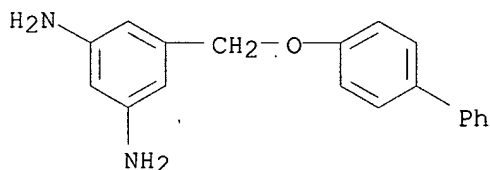
OTHER SOURCE(S): CASREACT 124:202946; MARPAT 124:202946

AB AX(CH<sub>2</sub>)<sub>m</sub>B(CH<sub>2</sub>)<sub>p</sub>XA [A = sugar alc. residue (derivative), tris(hydroxymethyl)methyl; ≥1 of the A OH groups are esterified with H<sub>2</sub>SO<sub>4</sub>; jX = NR<sub>1</sub>CO, NHCONH, NHCSNH, NHSO<sub>2</sub>, NR<sub>1</sub>, O; m, p = 0, 1; R<sub>1</sub> = H, alkyl, hydroxyalkyl; B = system of conjugated multiple bonds], were prepared. Thus, (Z)-3-[3-biphenyl-4-yloxymethyl-5-[(Z)-3-carboxyacryloylamino]phenylcarbamoyle]acrylic acid in DMF was treated successively with 4-methylmorpholine, 2-chloro-4,6-dimethoxy-1,3,5-triazine, and D-glucamine to give (Z)-butenedioic acid (Z)-[3-biphenyl-4-yloxymethyl-5-(3-D-glucit-1-ylcarbamoyle]acryloylamino]phenylamide]-D-glucit-1-ylamide, which was converted to (Z)-butenedioic acid (Z)-[3-biphenyl-4-yloxymethyl-5-[3-(2,3,4,5,6-penta-O-sulfo-D-glucit-1-ylcarbamoyle]acryloylamino]phenylamide]- (2,3,4,5,6-penta-O-sulfo-D-glucit-1-yl)amide. The latter had 2.2 times the antiproliferative activity of heparin without showing appreciable anticoagulative activity.

IT 171240-34-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of sulfate esters of sugar alcs. for the treatment of arteriosclerotic changes in the vascular walls)

RN 171240-34-9 CAPLUS

CN 1,3-Benzenediamine, 5-[[[1,1'-biphenyl]-4-yloxy)methyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:469544 CAPLUS

DOCUMENT NUMBER: 117:69544

TITLE: Calixarenes. 27. Synthesis, characterization, and complexation studies of double-cavity calix[4]arenes

AUTHOR(S): Gutsche, C. David; See, Keat Aun

CORPORATE SOURCE: Dep. Chem., Texas Christian Univ., Fort Worth, TX, 76129, USA

SOURCE: Journal of Organic Chemistry (1992), 57(16), 4527-39  
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:69544

AB The ease with which calix[4]arenes can be selectively substituted at the distal phenolic oxygens is employed to advantage to build a second cavity and create two classes of "double-cavity calixarenes". Through the use of 3,5-dinitrobenzoyl chloride, 3-nitro-5-carbomethoxybenzoyl chloride, 3,5-dinitrobenzyl chloride, or 3-nitro-5-carbomethoxybenzyl chloride and 4-tert-butylcalix[4]arene diesters, diether and ether-ester derivs. were prepared. The second cavity is built by reduction of the nitro groups to amino groups [e.g. of 5,11,17,23-tetra-tert-butyl-25,27-bis[(3,5-dinitrobenzyl)oxy]-26,28-dihydroxycalix[4]arene] to give amines, followed by treatment with a diacyl chloride. The products thus obtained are double-spanned double-cavity calix[4]arenes. A study of the complexation

characteristics of the double-spanned double-cavity calixarenes shows the diester double-cavity calix[4]arene to be effective in forming complexes with acidic compds. (i.e., phenols and carboxylic acids) as well as basic compds. (i.e., pyridines, imidazoles, aliphatic amines). The Kassoc values range from <5 to 55 M<sup>-1</sup> and are dependent both on the shape and the acidity or basicity of the guest. Several lines of evidence, including mol. modeling studies, indicate that complexation occurs at the side rather than the bottom of the host mol., providing an explanation for the differences in Kassoc for various pairs of guests and also establishing a rationale for the synthesis of the single-spanned double-cavity calix[4]arenes which form quite strong complexes (Kassoc > 103) with certain guests such as resorcinol.

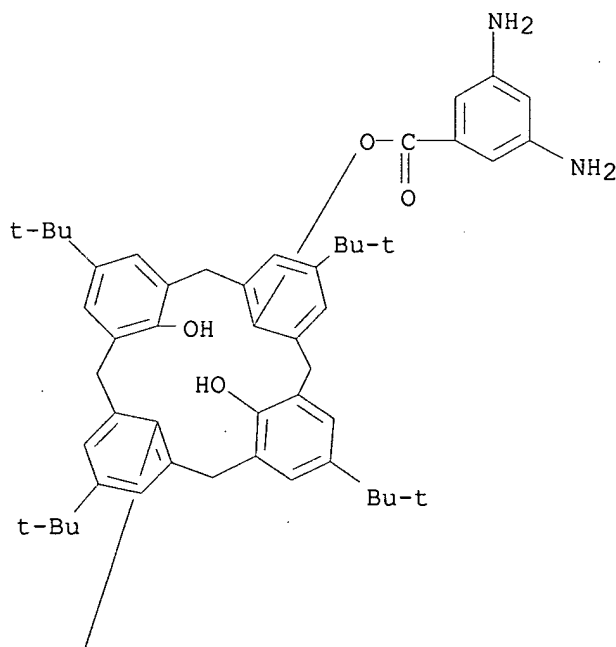
IT 142320-22-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and acylation of)

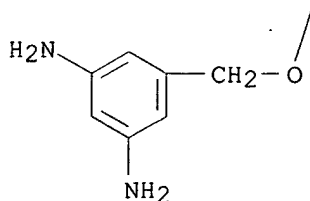
RN 142320-22-7 CAPLUS

CN Benzoic acid, 3,5-diamino-, 27-[(3,5-diaminophenyl)methoxy]-5,11,17,23-tetrakis(1,1-dimethylethyl)-26,28-dihydroxypentacyclo[19.3.1.13,7.19,13.11 5,19]octacosa-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaen-25-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IT 142319-83-3P

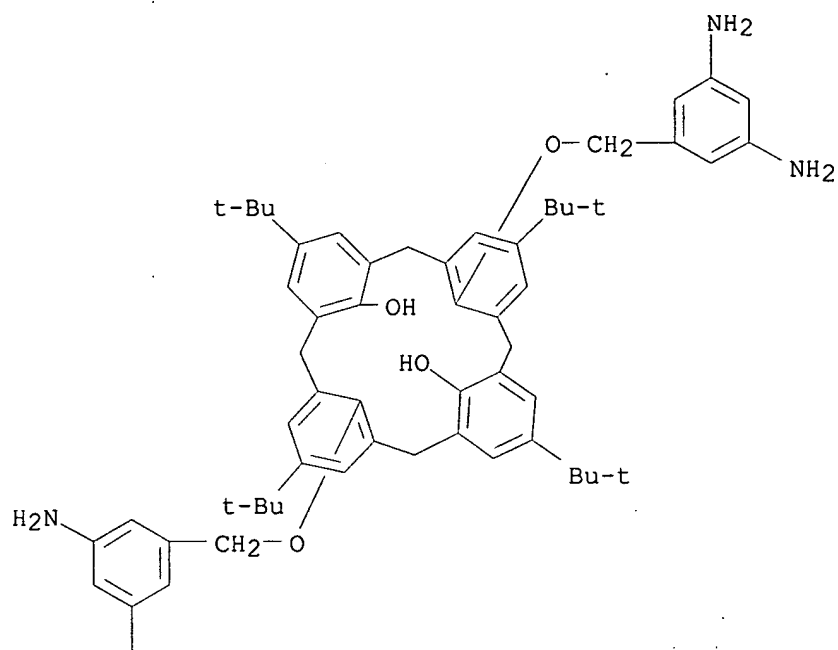
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and acylation of, double-spanned double-cavity calixarene from)

RN 142319-83-3 CAPLUS

CN Pentacyclo[19.3.1.13,7.19,13.115,19]octacos-1(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene-25,27-diol, 26,28-bis[(3,5-diaminophenyl)methoxy]-5,11,17,23-tetrakis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

NH<sub>2</sub>